
ACCORD: Autoregressive Constraint-satisfying Generation for COmbinatorial Optimization with Routing and Dynamic attention

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Abstract

Large Language Models (LLMs) have demonstrated impressive reasoning capabilities, yet their direct application to NP-hard combinatorial problems (CPs) remains underexplored. In this work, we systematically investigate the reasoning abilities of LLMs on a variety of NP-hard combinatorial optimization tasks and introduce **ACCORD**: Autoregressive Constraint-satisfying generation for **CO**mbinatorial optimization with **R**outing and **D**ynamic attention. **ACCORD** features a novel dataset representation and model architecture that leverage the autoregressive nature of LLMs to dynamically enforce feasibility constraints, coupled with attention-based routing to activate problem-specific LoRA modules. We also present the **ACCORD-90k** supervised dataset, covering six NP-hard combinatorial problems: TSP, VRP, Knapsack, FlowShop, JSSP, and BinPacking. Extensive experiments demonstrate that our **ACCORD** model, built on an 8B-parameter Llama backbone, consistently outperforms standard prompting and input-output methods, even when compared to much larger LLMs, such as gpt-4. Ablation studies further show that our output structure enhances solution feasibility. To the best of our knowledge, this is the first large-scale, end-to-end framework for exploring the applications of LLMs to a broad spectrum of combinatorial optimization problems. The codes are publicly available at ¹

1 Introduction

Large Language Models (LLMs) have rapidly established themselves as versatile engines for reasoning across a broad spectrum of tasks, encompassing arithmetic, commonsense logic, [27], [7], [6]. Among the prominent strategies enabling such capabilities is the Chain-of-Thought approach, which allows these models to decompose complex problems into sequential, interpretable steps [31].

Recent efforts have sought to adapt these reasoning techniques to address more advanced optimization tasks. Combinatorial optimization problems (CPs) are decision-making challenges where the goal is to select an optimal arrangement or subset from a large, discrete set of possibilities. Classic examples include the Traveling Salesman Problem (TSP), Vehicle Routing Problem (VRP), and Job Shop Scheduling Problem (JSSP), which have widespread applications in logistics, manufacturing, and artificial intelligence [18]. Due to their NP-hard nature, even moderately sized instances possess a combinatorial explosion of potential solutions, rendering brute-force approaches infeasible. As a result, practical methods typically rely on heuristics or approximation algorithms to provide near-optimal solutions within reasonable time frames. As NP-hard problems, CPs present huge obstacles in practical settings [24]. Presently, the predominant paradigm in industry relies on metaheuristic

¹<https://github.com/starjob42/ACCORD>

algorithms—sophisticated combinations of simple, efficient heuristics—for solving CPs under various constraints. However, the success of these heuristics is often highly sensitive to the specific structure and requirements of each problem, necessitating tailored approaches for optimal results.

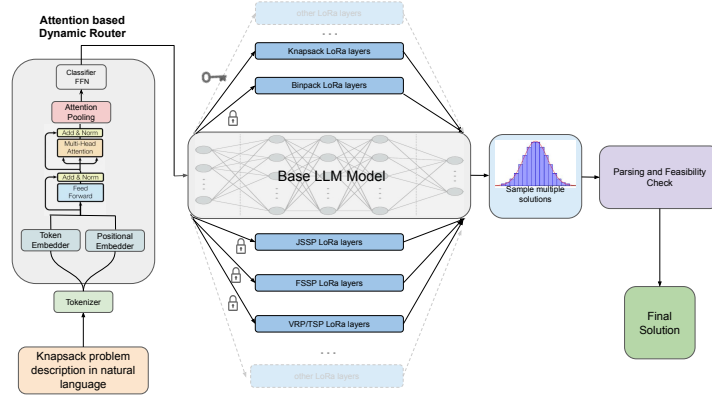


Figure 1: Overview of the ACCORD inference pipeline. As an example, a knapsack problem described in natural language is provided as input, then Attention based Dynamic router³ activates the corresponding LoRA layer specialized for knapsack tasks. Multiple candidate solutions are generated via sampling, each checked for feasibility. The best feasible solution is returned as the final output. Note that the pipeline generalizes to other combinatorial problems in the same manner; knapsack is shown here for illustration.

At the same time, investigations into leveraging LLMs for combinatorial problem solving have revealed significant research gaps. While the latest breakthroughs highlight the promise of LLMs in diverse reasoning scenarios [1], [14], [30], [34], their full potential in the context of combinatorial optimization remains largely untapped. Applying LLMs directly to these problems presents unique challenges: LLMs are trained primarily for natural language generation, not for enforcing strict combinatorial constraints, leading to issues such as hallucinations (plausible but infeasible solutions) [12], lack of optimality, and limited interpretability [28]. Furthermore, the absence of systematic search or explicit constraint mechanisms means LLM outputs can violate feasibility or fail to improve upon prior attempts. Recent advances have begun to explore the application of large language models (LLMs) to combinatorial optimization (CO). Numerous prompting-based approaches have been tested on CO tasks [32, 13, 22, 31, 35, 20, 14], demonstrating progress in solution quality and constraint handling. However, to date, there has been no comprehensive study evaluating a unified fine-tuned LLM-based framework for NP-hard CO problems across multiple domains.

We introduce **ACCORD** (Autoregressive Constraint-satisfying generation for **CO**mbinatorial optimization with **R**outing and **D**ynamic attention), a framework for evaluating LLMs on combinatorial optimization. Our contributions are: (i) the ACCORD-90k dataset for TSP, VRP, Knapsack, FlowShop, JSSP, and BinPacking, using an autoregressive constraint-aware representation; (ii) a model architecture with attention-based dynamic routing and task-specific LoRA modules; (iii) extensive ablations showing lower optimality gaps and higher feasibility than list-of-lists and SOTA prompting (e.g., GPT-4 with Code Interpreter). ACCORD yields feasibility gains of 24.86% (FlowShop), 10% (TSP, VRP), 7% (JSSP), 4% (Knapsack), and 2% (BinPacking). This is the first large-scale, end-to-end CO framework with LLMs, opening new directions in symbolic reasoning and optimization.

2 Main Method: ACCORD Representation for Feasibility-Aware Solution Generation

A core challenge in applying Large Language Models (LLMs) to combinatorial optimization is the effective encoding of feasibility constraints within the generated solutions. Conventional representations, such as the “list of lists” format, provide direct encodings of solution sets, which are familiar to LLMs due to their prevalence in general-purpose data and code corpora. However, these representations are static—constraints are only checked after solution generation, offering limited guidance for incremental feasibility during the autoregressive decoding process. To address this limi-

Table 1: Optimality gap (%) of prompting methods (GPT-4 with code interpreter) vs. ACCORD (Llama 8B). Lower is better. N/A: no feasible solution.

Size	Method	Knapsack	BinPack	TSP	VRP	JSSP
5	IO (GPT-4)	90.1	108.2	100.3	102.0	105.3
	CoT (GPT-4)	66.9	78.2	81.2	78.2	79.4
	SR (GPT-4)	62.0	77.4	71.6	72.5	71.7
	LtM (GPT-4)	21.6	40.0	43.6	40.7	44.1
	SGE (GPT-4)	8.1	9.1	8.3	11.9	9.3
	IO (Llama 8B)	N/A	N/A	N/A	N/A	N/A
	ACCORD (Llama 8B)	3.9*	0.0*	0.6*	1.0*	0.0*
8	IO (GPT-4)	103.5	112.8	116.9	116.3	108.2
	CoT (GPT-4)	73.8	85.1	89.0	89.5	85.2
	SR (GPT-4)	72.6	86.3	85.6	83.3	78.4
	LtM (GPT-4)	26.4	52.7	53.5	54.4	49.8
	SGE (GPT-4)	14.9	21.0	15.2	19.7	21.3
	IO (Llama 8B)	N/A	N/A	N/A	N/A	N/A
	ACCORD (Llama 8B)	7.4*	0.0*	1.8*	1.0*	5.0*
12	IO (GPT-4)	101.5	120.7	121.6	118.5	117.6
	CoT (GPT-4)	79.3	93.8	86.8	90.1	89.3
	SR (GPT-4)	77.1	82.2	88.6	88.4	87.0
	LtM (GPT-4)	35.8	55.4	57.5	59.2	56.0
	SGE (GPT-4)	16.8	22.4	16.1	24.0	22.9
	IO (Llama 8B)	N/A	N/A	N/A	N/A	N/A
	ACCORD (Llama 8B)	5.1*	2.6*	2.9*	2.2*	12.4*

tation, we decided to utilize the auto-regressive nature of the LLMs and developed a representation, which is specifically designed to leverage the autoregressive generation paradigm of LLMs. Unlike the list-based format, our representation decomposes solutions into a sequence of state transitions, with each step not only specifying the next element of the solution but also explicitly updating and exposing the relevant feasibility metrics (e.g., cumulative weights, distances, machine usage, or value). This design allows the model to compute and check constraints dynamically as each token is generated, closely mimicking the typical reasoning and verification process of a human solver. ACCORD representation embeds constraint satisfaction directly into the generation process. For instance, in the Knapsack problem, each item addition is accompanied by an explicit update of the running total value and weight, immediately verifying the capacity constraint at each step:

```
[[item_id, weight, value] -> value: prev_v + value = new_v,
weight: prev_w + weight = new_w <= capacity], ...
```

Please refer to page 1 in Appendix A for a concrete example. Similarly, for Bin Packing, the incremental assignment of items to bins is annotated with cumulative weights, ensuring that no bin exceeds its capacity as the sequence unfolds. Routing problems (VRP, TSP) and scheduling problems (JSSP) are analogously handled by tracking cumulative distances or machine times within the autoregressive output stream. Example of each of these generators is available in the Appendix A. This approach transforms the constraint satisfaction problem into a stepwise process, where feasibility checks are interleaved with generation. As a result, the LLM is naturally guided away from infeasible sequences, as each decision is immediately contextualized by the current state of the solution.

2.1 Dataset Generation

We generated synthetic datasets for several CO problems using Google OR-Tools [10], producing about 15,000 instances per task in both list-of-lists and ACCORD formats. **TSP & VRP:** Instances varied by location count ($N \in \{5, \dots, 100\}$) and vehicles ($V \in \{1, \dots, 10\}$), solved via 'PATH_CHEAPEST_ARC'. **Knapsack:** Varied item counts and constraints; instances with OR-Tools timeouts were discarded. **Bin Packing:** Item counts, weights, and bin limits were randomized; solutions minimized bin usage. **JSSP:** Instances ranged from 10×10 to 100×20 with random job sequences, solved via CP-SAT. **FSSP:** Flowshop instances up to 50×2 used the NEH heuristic [23]. See Appendix D for details.

3 Model Architecture

To dynamically activate the correct LoRA layers for each combinatorial optimization problem, we use an attention-based Dynamic Router TextClassifier that selects the appropriate LoRA weights

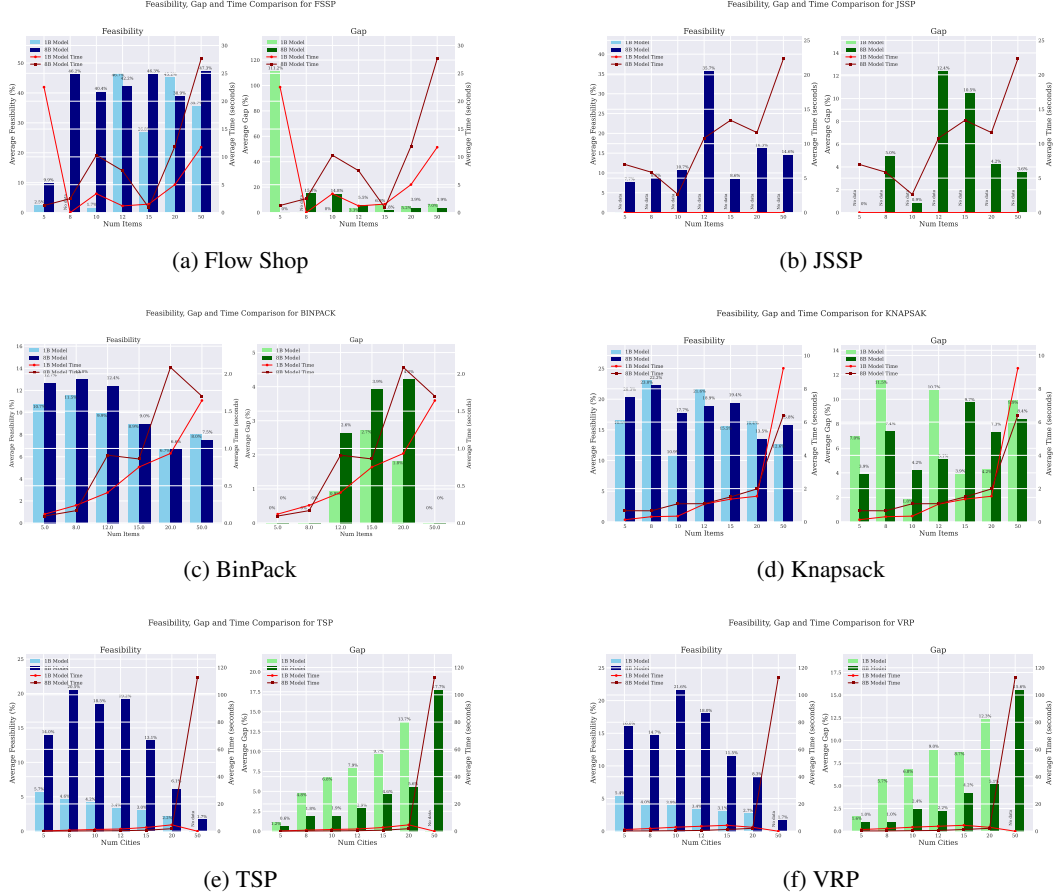


Figure 2: This figure illustrates the performance of the LLama 3.1 (8B) and LLama 3.2 (1B) models in terms of the average gap percentage compared to the OR-Tools solution, where a lower gap indicates better performance. The left y-axis represents the average gap percentage, while the right y-axis corresponds to the running time in seconds. Bar plots indicate the average gap. The line plots depict the average running time per instance size, with the x-axis showing the problem size in terms of the number of nodes in the graph representation. Instances labeled as "No Data" indicate that, within a sampling budget of 60, the model failed to generate any feasible solution.

99 based on the instruction text (see Figure 1). Our model builds on a transformer architecture, enhanced
100 to capture problem-specific features. Each input token x_i is embedded with positional information
101 and normalized:

$$\mathbf{E}' = \text{Dropout}(\text{LayerNorm}(\mathbf{E}_{\text{token}}(\mathbf{x}) + \mathbf{E}_{\text{pos}}(\mathbf{p}))) \quad (1)$$

102 The embeddings are projected to the hidden dimension and passed through several transformer
103 layers with alternating multi-head attention and feed-forward sublayers, each followed by layer
104 normalization. Token representations from the final transformer layer are pooled using attention-
105 based pooling:

$$\mathbf{r} = \sum_{i=1}^n a_i \mathbf{h}_i \quad \mathbf{y} = \mathbf{W}_2 \cdot \text{LayerNorm}(\text{GELU}(\mathbf{W}_1 \mathbf{r} + \mathbf{b}_1)) + \mathbf{b}_2 \quad (2)$$

106 Finally, the pooled vector $\mathbf{r}$ is passed through a classification head to produce logits $\mathbf{y}$ for each
107 problem class. This architecture enables dynamic, instruction-based activation of problem-specific
108 LoRA adapters.



Figure 3: Average feasibility comparison with OR-Tools solution across different problem instance sizes; the higher the feasibility percentage, the better.

3.1 Empirical Comparison with List-of-List Representation

We assess representation impact by fine-tuning LLaMA 3.1 8B on both list-of-lists and ACCORD formats using identical hyperparameters and inputs (Section 2.1). Validation uses 100 out-of-distribution instances for each $n \in \{5, 8, 10, 12, 15, 20, 25, 30, 50\}$. During inference (Fig. 1), an Attention-Based Dynamic Router (Section 3) selects the LoRA branch, generating 60 candidate solutions per instance. The best feasible solution (lowest gap) is selected, where the optimality gap is defined as $\text{Gap} = \frac{\text{Model Value} - \text{OR-Tools Value}}{\text{OR-Tools Value}}$.

where a lower gap indicates a better solution. Feasibility is measured as the percentage of generated solutions that satisfy all constraints. Our results (Fig. 3) show that, although list-of-list representation is familiar to LLMs, models trained with this format tend to ignore feasibility constraints, resulting in lower feasibility rates and higher optimality gaps. In contrast, the ACCORD representation explicitly encodes feasibility into the output, enabling the LLM to produce a larger proportion of valid and near-optimal solutions, particularly as the problem size increases. Table 1 further compares our method against various prompting strategies (see Section B for baselines) on both LLaMA 8B and GPT-4 with code interpreter enabled. Notably, while GPT-4 can potentially generate and execute solver code, our ACCORD-based method enables the LLM to generate solutions end-to-end without code execution. For both our approach and all prompting baselines, 60 samples per instance are generated, and the best result is selected. ACCORD consistently outperforms prompting strategies across all 6 combinatorial optimization tasks, and achieves optimal solutions on smaller instances. We also assess the impact of model size on average gap, feasibility, and inference time (Fig. 2). The 8B model mostly outperforms the 1B model in feasibility and optimality gap, with only a moderate increase in inference time. For harder instances, such as JSSP, the 1B model fails to find feasible solutions within the sampling limit. Our results demonstrate that scaling from 1B to 8B parameters

132 yields a significant 31.5% relative improvement in solution quality, reducing the average gap from
 133 6.54% to 4.48% (Table 2). The most substantial improvements were observed in routing problems,
 134 with TSP and VRP showing 65% and 54% relative gap reductions, respectively. Bin packing problems
 135 showed minimal sensitivity to model scale, with only a 1% improvement. In addition to our synthetic
 136 OR-Tools instances, we also evaluated ACCORD-8B on Taillard permutation flow-shop benchmarks
 137 (50 jobs $\times$ 10 machines and 50 jobs $\times$ 20 machines; avg. gap $\approx$ 13.7%) and on job-shop benchmarks
 138 TAI[26] (15 $\times$ 15 to 50 $\times$ 20; avg. gap $\approx$ 21.7%) and DMU[8] (20 $\times$ 15 to 50 $\times$ 15; avg. gap $\approx$ 22.1%)
 139 against standard heuristics (MWR/MOR/SPT) and the L2D neural scheduler (see Supplementary
 140 Material for full results and runtimes).

141 3.2 Relationship Between Latent Space Proximity and Solution Feasibility

142 We analyzed 500 TSP instances using ACCORD and list-of-lists formats to study how latent represen-
 143 tations relate to solution feasibility. Hidden states from LLaMA 3.1 8B were reduced via PCA, and
 144 Euclidean distances between paired representations were computed. We found a significant negative
 145 correlation between latent distance and feasibility ($r = -0.1082$, $p = 0.0155$), with feasibility
 146 decreasing as distance from the ACCORD manifold increased. Despite a large performance gap
 147 (71.4% feasible for ACCORD vs. 1.6% for list-of-lists), this trend suggests LLMs encode constraint
 148 satisfaction geometrically, with latent proximity predicting solution quality.

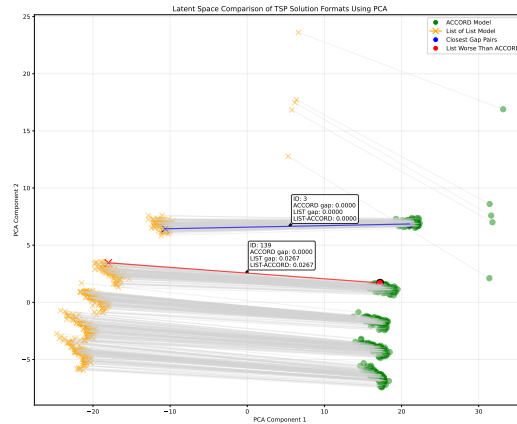


Figure 4: Latent representation distance versus solution feasibility on TSP problems, demonstrating negative correlation between distance and constraint satisfaction.

149 4 Conclusion, Limitations and Future Work

150 We introduced ACCORD, a framework that encodes combinatorial constraints into an autoregressive
 151 text format and uses dynamic LoRA routing to probe an LLM’s end-to-end ability on NP-hard tasks.
 152 On six standard benchmarks (TSP, VRP, FlowShop, JSSP, Knapsack, BinPacking), an 8 B-parameter
 153 model trained with ACCORD achieves strong feasibility rates and competitive optimality gaps
 154 compared to prompting and a naïve list-of-lists format. Our goal is not to supplant specialized solvers
 155 but to map out how far small LLMs can go as self-contained combinatorial reasoners. By releasing
 156 ACCORD and its 90K dataset, we offer a reproducible codebase for future work at the intersection
 157 of optimization and generative modeling. Despite its strong performance, ACCORD is bounded
 158 by the LLM’s context window (limiting very large instances) and relies on LoRA adapters on an
 159 8B-parameter model. In future work, we will investigate larger backbones (with full fine-tuning),
 160 expand the effective context via external memory or hierarchical encoding, and apply ACCORD to
 161 real-world, large-scale optimization scenarios.

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A Technical Appendices and Supplementary Material

B Related Work

B.1 Heuristic and Machine Learning Approaches on CO problems

Combinatorial optimization has been tackled with both heuristic and exact methods. Simple priority dispatching rules (PDRs), such as shortest processing time or earliest due date, are computationally efficient but often yield suboptimal solutions due to their greedy nature [18]. Metaheuristics (e.g., simulated annealing, tabu search, genetic algorithms) offer improved solution quality, and exact approaches like the shifting bottleneck procedure [2], mixed-integer programming, and constraint programming can find optimal solutions for small instances, though at high computational cost [25, 9]. Recently, machine learning, particularly deep reinforcement learning (RL) and graph neural networks (GNNs) have advanced combinatorial optimization [33, 16, 17]. RL methods treat scheduling as sequential decision making, learning dispatching policies via environment interaction [33]. GNNs encode jobs and machines as nodes, enabling permutation-invariant representations and, when combined with RL, can model complex dependencies [16]. Attention-based and sequence-to-sequence models further enhance performance on tasks like TSP and VRP, often utilizing iterative refinement [17].

B.2 Large Language Models in Combinatorial Optimization

The advent of LLMs has introduced new paradigms for CO. Early work explored whether LLMs could generate solutions through prompting [32], [13], [22], [31] [35], [20], [14]. Prompting-based strategies, such as OPRO, involve iterative refinement based on feedback, while methods for VRP employ self-debugging and verification to enhance feasibility [13]. However, scalability remains a challenge, as even strong prompting techniques struggle on larger or more complex instances [22]. Recent research has explored a variety of prompting strategies to leverage LLMs for solving combinatorial optimization (CO) problems. The **Input-Output (IO)** method presents the LLM with multiple examples of input and corresponding output solution pairs. The LLM is then prompted to generate an output solution in the same format as the provided examples. This approach relies on the LLM’s ability to generalize the mapping from input to output based on observed patterns. In **Chain-of-Thought (CoT)** prompting, the LLM is guided to produce a sequence of intermediate reasoning steps, or “thoughts,” before arriving at the final answer [31]. This technique encourages the model to break down complex CO tasks into structured, stepwise reasoning, improving both transparency and solution quality. **Least-to-Most (LtM)** prompting strategy aims to decompose a complex problem into a sequence of simpler subproblems, solving them incrementally [35]. Each subproblem builds upon the solutions of previous ones, enabling the LLM to tackle challenging CO tasks through a series of manageable steps. **Self-Refinement (SR)** is an iterative prompting technique wherein the LLM first generates an initial solution, then provides feedback on its own output, and finally refines the solution based on this feedback [20]. The process repeats until a satisfactory solution is reached. **Self-Guiding Exploration for Combinatorial Problems (SGE)** autonomously generates multiple thought trajectories for a given CO task [14]. Each trajectory represents a distinct heuristic approach, inspired by metaheuristics. SGE decomposes these trajectories into actionable subtasks, executes them sequentially, and refines the results to ensure optimal solutions. Fine-tuning LLMs for CO tasks is another active area [1],[21] . [1] showed that fine-tuned LLM on job-shop scheduling, demonstrates significant improvements in solution quality. Similarly, [21] applied fine-tuning to TSP instances with promising but size-limited results. Hybrid methods integrate LLMs into evolutionary or search frameworks, where the LLM guides genetic operations or receives feedback from constraint solvers to iteratively improve solutions [19, 29, 5]. While promising, these approaches often entail significant computational overhead and still face scaling hurdles.

C Preliminaries: Overview of Classic Combinatorial Optimization Problems

In this section, we introduce several foundational combinatorial optimization problems, explaining their goals and constraints in accessible terms while also providing their standard mathematical formulations. **General Combinatorial Optimization Problem** Combinatorial optimization involves searching for the best solution from a finite set of possibilities. Formally, given a set of feasible

300 solutions $\mathcal{S}$ and an objective function $f : \mathcal{S} \rightarrow \mathbb{R}$, the goal is to find

$$s^* = \arg \min_{s \in \mathcal{S}} f(s)$$

301 or, in some cases, to maximize $f(s)$ depending on the problem.

302 **Traveling Salesman Problem (TSP)** Given a list of cities and the distances between each pair of
 303 cities, what is the shortest possible route that visits each city exactly once and returns to the starting
 304 point. Mathematically, for n cities $V = \{1, 2, \dots, n\}$ and a distance matrix $D \in \mathbb{R}^{n \times n}$, we seek a
 305 tour (a permutation π of all cities) that minimizes the total travel distance, where $\pi(n+1) = \pi(1)$ to
 306 ensure the tour closes:

$$\min_{\pi \in \mathcal{P}_n} \sum_{i=1}^n D_{\pi(i), \pi(i+1)}$$

307 **Vehicle Routing Problem (VRP)** The VRP extends the TSP to multiple vehicles. Given a depot,
 308 n customers (with demands q_i), and a fleet of vehicles each with capacity Q , the goal is to design
 309 routes—each starting and ending at the depot—so that every customer is visited exactly once, no
 310 vehicle exceeds its capacity, and the total travel distance is minimized:

$$\min \sum_{k=1}^m \sum_{j=0}^{\ell_k} D_{v_j^k, v_{j+1}^k}$$

311 subject to

$$\begin{aligned} \bigcup_{k=1}^m \{v_1^k, \dots, v_{\ell_k}^k\} &= V \quad (\text{All customers served}) \\ \sum_{j=1}^{\ell_k} q_{v_j^k} &\leq Q \quad \forall k \quad (\text{Capacity constraint}) \end{aligned}$$

312 **Job Shop Scheduling Problem (JSSP)** JSSP schedules n jobs, each as a sequence of operations
 313 on specific machines. Each operation $O_{j,k}$ requires machine $M_{j,k}$ for $p_{j,k}$ time units, following job
 314 order. Let $S_{j,k}$ and $C_{j,k}$ be the start and completion times. The objective is to minimize makespan:

$$\min C_{\max} = \max_j C_{j, \ell_j}$$

315 subject to:

$$\begin{aligned} (\text{Precedence}) \quad & S_{j,k+1} \geq C_{j,k} \\ (\text{No machine conflicts}) \quad & S_{j,k} \geq C_{j',k'} \text{ or } S_{j',k'} \geq C_{j,k}, \\ & \forall (j,k) \neq (j',k') \text{ with } M_{j,k} = M_{j',k'} \end{aligned}$$

316 **Knapsack Problem (KP)** Given a set of items, each with a value and weight, what is the most
 317 valuable combination of items you can carry without exceeding the weight limit of your knapsack.
 318 With n items (weights w_i , values v_i) and capacity W , choose $x_i \in \{0, 1\}$ (item picked or not) to
 319 solve:

$$\max \sum_{i=1}^n v_i x_i \quad \text{s.t.} \quad \sum_{i=1}^n w_i x_i \leq W$$

320 **Bin Packing Problem (BPP)** Given a set of items of varying sizes, how can you pack them into the
 321 fewest number of fixed-size bins. For n items of sizes $s_i \in (0, 1]$, assign them to bins of capacity 1
 322 so as to minimize the total number of bins K :

$$\min K$$

323 subject to:

$$\sum_{i \in B_k} s_i \leq 1 \quad \forall k, \quad \bigcup_{k=1}^K B_k = \{1, \dots, n\}, \quad B_k \cap B_{k'} = \emptyset \quad \forall k \neq k'$$

324 where B_k is the set of items in bin k .

325 Flow Shop Scheduling Problem (FSSP)

326 We consider the permutation flow shop scheduling problem (FSSP), where all jobs are processed in
 327 the same order on each of m machines. Given n jobs $J = \{1, 2, \dots, n\}$ and processing times $p_{j,k}$
 328 for job j on machine k , the goal is to find a job sequence π that minimizes the makespan.

329 Let $C_{j,k}$ denote the completion time of job j on machine k . The constraints are:

$$\text{(Machine order)} \quad C_{\pi(i),k} \geq C_{\pi(i),k-1} + p_{\pi(i),k} \quad \forall i = 1, \dots, n, k = 2, \dots, m$$

$$\text{(Job sequence)} \quad C_{\pi(i),k} \geq C_{\pi(i-1),k} + p_{\pi(i),k} \quad \forall i = 2, \dots, n, k = 1, \dots, m$$

330 The objective is to find the permutation π^* that minimizes the makespan:

$$\min_{\pi \in \mathcal{P}_n} C_{\max} = \min_{\pi \in \mathcal{P}_n} \max_i C_{\pi(i),m}$$

331 where $C_{\pi(i),m}$ is the completion time of job $\pi(i)$ on the last machine.

332 Below, we provide representative examples from each of the major combinatorial optimization
 333 problems in our dataset. Each example is shown in both the standard “list of list” representation and
 334 the “Accord” (arrow-based) representation.

335 Knapsack Problem

336 **Instruction:** You are given a paired representation (value, weight): Find a set of items to pack into a
 337 container with a maximum weight capacity = 20 that maximizes total value of packed items.

338 • **Input:**

$$\begin{bmatrix} 6 & 5 \\ 10 & 8 \\ 7 & 4 \\ 6 & 2 \\ 1 & 1 \end{bmatrix}$$

339 • **Output (List of List):**

340 Solution: [(6, 5), (10, 8), (7, 4), (6, 2), (1, 1)]

341 Value: 6+10+7+6+1=30

342 Weight: 5+8+4+2+1=20<=20

343

344 • **Output (Accord):**

345 Solution:

346 [[6, 5] -> value:0+6=6, weight:0+5=5<=20],

347 [[10, 8] -> value:6+10=16, weight:5+8=13<=20],

348 [[7, 4] -> value:16+7=23, weight:13+4=17<=20],

349 [[6, 2] -> value:23+6=29, weight:17+2=19<=20],

350 [[1, 1] -> value:29+1=30, weight:19+1=20<=20]

351

352 Total Value: 30

353 Total Weight: 20<=20

354

355 Bin Packing Problem

356 **Instruction:** Given a list of items (id, weight), determine the minimum number of bins (capacity=77)
 357 needed to pack all items without exceeding the capacity.

358 • **Input:**

$$[(0, 17), (1, 24), (2, 19), (3, 11), (4, 27)]$$

359 • **Output (List of List):**

360 The minimum number of bins required is 2. The bin assignments are: [[0, 1, 2, 3], [4]].

361

362 • **Output (Accord):**

363 Bin 1:

364 (0, 17)->17 (1, 24)->41 (2, 19)->60 (3, 11)->71<=77

365 Bin 2:

366 (4, 27)->27<=77

367 Total bins required: 2

368

369 **Vehicle Routing Problem (VRP)**

370 **Instruction:** Given customers with coordinates and a depot, and multiple vehicles of capacity 85,

371 find the minimum-length routes serving all customers.

372 • **Coords:** 0:(34, 42), 1:(39, 58), 2:(46, 48), 3:(57, 49), 4:(45, 16)

373 • **Output (List of List):**

374 [(0): (34, 42), (0): (34, 42)]

375 [(0): (34, 42), (0): (34, 42)]

376 [(0): (34, 42), (0): (34, 42)]

377 [(0): (34, 42), (0): (34, 42)]

378 [(0): (34, 42), (1): (39, 58), (2): (46, 48),

379 (3): (57, 49), (4): (45, 16), (0): (34, 42)]

380 Overall Total Distance: 102

381

382 • **Output (Accord):**

383 Vehicle Route: (0): (34, 42) -> (0): (34, 42) + 0

384 Vehicle Route: (0): (34, 42) -> (0): (34, 42) + 0

385 Vehicle Route: (0): (34, 42) -> (0): (34, 42) + 0

386 Vehicle Route: (0): (34, 42) -> (0): (34, 42) + 0

387 Vehicle Route: (0): (34, 42) -> (1): (39, 58) + 16 -> (2): (46, 48) + 12 ->

388 (3): (57, 49) + 11 -> (4): (45, 16) + 35 -> (0): (34, 42) + 28

389 Overall Total Distance: 102

390

391 **Traveling Salesman Problem (TSP)**

392 **Instruction:** Given customers with coordinates and a depot, and 1 vehicle, find the minimum-length

393 route serving all customers.

394 • **Coords:** 0:(17, 22), 1:(63, 8), 2:(22, 60), 3:(3, 29), 4:(7, 12)

395 • **Output (List of List):**

396 [(0): (17, 22), (4): (7, 12), (3): (3, 29), (2): (22, 60), (1): (63, 8), (0): (17, 22)]

397 Overall Total Distance: 181

398

399 • **Output (Accord):**

400 Vehicle Route: (0): (17, 22) -> (4): (7, 12) + 14 -> (3): (3, 29) + 17 ->

401 (2): (22, 60) + 36 -> (1): (63, 8) + 66 -> (0): (17, 22) + 48

402 Overall Total Distance: 181

403

404 **Job Shop Scheduling Problem (JSSP)**

405 **Instruction:** Optimize schedule for 2 Jobs (J) across 6 Machines (M) to minimize makespan. Each

406 M can process only one J at a time, and once started, J cannot be interrupted.

```

407     • Input:
408         J0:
409         M2:205 M1:157 M0:198 M5:79 M3:110 M4:32
410         J1:
411         M3:179 M4:108 M2:82 M5:112 M1:136 M0:27
412
413     • Output (List of List):
414         [[0, 2, 0, 205], [1, 3, 0, 179], [1, 4, 179, 108], [0, 1, 205, 157], [1, 2, 287, 82],
415         [0, 0, 362, 198], [1, 5, 369, 112], [1, 1, 481, 136], [0, 5, 560, 79], [1, 0, 617, 27],
416         [0, 3, 639, 110], [0, 4, 749, 32]]
417         Maximum end completion time or Makespan: 781
418
419     • Output (Accord):
420         Solution:
421         J0-M2: 0+205 -> 205,
422         J1-M3: 0+179 -> 179,
423         J1-M4: 179+108 -> 287,
424         J0-M1: 205+157 -> 362,
425         J1-M2: 287+82 -> 369,
426         J0-M0: 362+198 -> 560,
427         J1-M5: 369+112 -> 481,
428         J1-M1: 481+136 -> 617,
429         J0-M5: 560+79 -> 639,
430         J1-M0: 617+27 -> 644,
431         J0-M3: 639+110 -> 749,
432         J0-M4: 749+32 -> 781,
433         Maximum end completion time or Makespan: 781
434
435 Flow Shop Scheduling Problem (FSSP)
436 Input:
437     J1:
438     M1:12 M2:7
439     J2:
440     M1:8 M2:4
441     J3:
442     M1:4 M2:15
443     J4:
444     M1:5 M2:9
445 Output (List of List):
446     [[3, 1, 0, 4], [3, 2, 4, 15], [2, 1, 4, 8], [4, 1, 12, 5],
447     [1, 1, 17, 12], [2, 2, 19, 4], [4, 2, 23, 9], [1, 2, 32, 7]]
448     Maximum end completion time or Makespan: 39
449 Output (Accord):
450     J3: M1(0+4=4) -> M2(4+15=19)
451     J2: M1(4+8=12) -> M2(19+4=23)
452     J4: M1(12+5=17) -> M2(23+9=32)
453     J1: M1(17+12=29) -> M2(32+7=39)
454
455     Maximum end completion time or Makespan: 39

```

D Training Details

We conducted supervised fine-tuning using input-output pairs for two models from Meta: Llama 3.1 8B and Llama 3.2 1B. To minimize memory usage during training, we employed 4-bit quantized versions of these models and trained each for 2 epochs. For a fair comparison, we fine-tuned each model with the same hyperparameters, varying only the output representation: once using the list-of-lists format and once using the ACCORD format, while keeping the input and all other hyperparameters identical. We used Rank-Stabilized Low-Rank Adaptation (RSLORA) [15] with a rank of $r = 64$ and $\alpha = 64$. The two epochs, training required roughly 40 hours and about 30GB of GPU memory on Nvidia RTX A6000 GPU. We limited the context length of the model to 40k instead of the original 128k, to reduce memory consumption and increase the speed of fine-tuning. “Context length” refers to the maximum number of tokens (words or subwords) the model can process at once as input. More training details and curves are available in D.

Training details

The model being fine-tuned is LLaMA 3.1, an 8 billion parameter model from Meta[3], using a 4-bit quantized version to reduce memory usage. Finetuning was conducted using Stabilized Low-Rank Adaptation (RsLoRA) [15] with rank $r = 64$ to introduce learnable parameters specifically in targeted layers. [15] Compared to Lora[11] RsLoRa improves the stability of training by modifying the rank during adaptation[15]. The target modules include:

$$\text{target_modules} = \{\text{q_proj}, \text{k_proj}, \text{v_proj}, \text{o_proj}, \text{gate_proj}, \text{up_proj}, \text{down_proj}\} \quad (3)$$

The LoRA-specific parameters are configured as follows:

- Rank (r): 64
- LoRA Alpha (α): 64
- LoRA Dropout: 0
- Bias: none

This resulted in number of trainable parameters = 167,772,160 or 0.02 % of the entire Llama 8B model’s parameters.

Quantization and Memory Efficiency

The model is loaded in 4-bit precision to reduce memory consumption. Gradient checkpointing is enabled using the `unsloth` [4] method, to fit longer sequences by saving memory. This reduces the VRAM usage by approximately 30%, enabling larger batch sizes.

Table 2: The effect of the model size on Average Gap (%): Comparison Across CO Problems

Problem	1B Model	8B Model
BINPACK	1.01%	1.00%
FSSP	7.92%	7.17%
JSSP	N/A	6.08%
KNAPSAK	5.90%	5.33%
TSP	8.11%	2.84%
VRP	9.74%	4.50%
AVERAGE	6.54%	4.48%

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- 813
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 - Please refer to our LLM policy (<https://neurips.cc/Conferences/2025/LLM>) for what should or should not be described.